$$\frac{\partial \psi}{\partial \tau} = \left(\frac{\kappa_{diff}}{\epsilon \alpha}\right)\left[\frac{1}{\frac{1}{\alpha} + \frac{\kappa_{ads}}{(1+\kappa_{ads}\psi)^2}}\right]\left[\frac{\partial^2 \psi}{\partial \lambda^2} - \phi^2 \frac{\psi}{(1+\kappa_{ads}\psi)^2}\right]$$

$\psi = \dfrac{C_A}{C_{A,max}}$ = gas-phase reactant concentration

$\tau = t(s)k_{-1}(s^{-1})$ = dimensionless time

where k_{-1} is the reactant desorption rate constant in step 1.

$\kappa_{diff} = \left(\dfrac{D_e}{L^2}\right)\left(\dfrac{1}{k_{-1}}\right)$ = dimensionless diffusion coefficient in layer of thickness L

$\kappa_{ads} = \dfrac{k_1(\text{m}^3\text{mol}^{-1}\text{s}^{-1})C_{A,max}(\text{mol m}^{-3})}{k_{-1}(\text{s}^{-1})}$ = reactant adsorption rate constant

$\kappa_{rxn} = \dfrac{k_2(\text{s}^{-1})}{k_{-1}(\text{s}^{-1})}$ = reaction rate constant

ϵ = void fraction in porous catalyst layer

$\alpha = \dfrac{A(\text{m}^2)C_{A,max}^{\text{surface}}(\text{mol m}^{-2})}{\epsilon V(\text{m}^3)C_{A,max}^{\text{gas}}(\text{mol m}^{-3})}$ = surface-to-gas capacity ratio

$\lambda = \dfrac{z(\text{m})}{L(\text{m})}$ = position within layer

Square of Thiele Modulus:

$$\phi^2 = \left(\frac{\kappa_{rxn}\kappa_{ads}}{\kappa_{diff}/(\epsilon\alpha)}\right) = \frac{L^2}{D_e}\left[k_2(A/V)\kappa_{ads}C_{A,max}^{\text{surface}}\right] = \frac{L^2(\text{m}^2)}{D_e(\text{m}^2\ \text{s}^{-1})}\left[K_r(\text{s}^{-1})\right]$$

At steady state: $\dfrac{\partial^2 \psi}{\partial \lambda^2} = \phi^2 \dfrac{\psi}{(1+\kappa_{ads}\psi)^2}$

$\theta_{AS} = \dfrac{\kappa_{ads}\psi}{1+\kappa_{ads}\psi}$ = local coverage of surface by adsorbed A ; local reaction rate = $\dfrac{\kappa_{rxn}\kappa_{ads}\psi}{(1+\kappa_{ads}\psi)^2}$

Match catalyst layer to mixing cell:

$$\left(\frac{V_{cell}}{V_{layer}}\right)\frac{d\psi_c}{d\tau} = \kappa_{flow}(\psi_{in}-\psi_c) - \kappa_{diff}\left[\frac{d\psi}{d\lambda}\right]_{\lambda=1} \quad \text{where } \psi_c = \text{reactant in mixing cell}$$

$$\kappa_{flow} = \frac{Q}{V_{layer}k_{-1}} = \frac{Q}{V_{cell}k_{-1}}\left(\frac{V_{cell}}{V_{layer}}\right) \quad \text{where } Q(\text{m}^3\ \text{s}^{-1}) = \text{flow rate through mixing cell}$$

Local reaction rate as dimensionless turnover frequency (TOF):

$$\text{local d'less TOF} = \frac{\text{mol A reacting}}{(\text{mol surface sites})(\text{dimensionless time})}$$

$$= \frac{\kappa_{rxn}\kappa_{ads}\psi}{(1+\kappa_{ads}\psi)^2}$$

Average reaction rate in catalyst layer as dimensionless turnover frequency (TOF):

$$\text{average d'less TOF} = \int_{\lambda=0}^{\lambda=1} \frac{\kappa_{rxn}\kappa_{ads}\psi}{(1+\kappa_{ads}\psi)^2}\,d\lambda$$

$$= \left(\frac{\kappa_{diff}}{\alpha\epsilon}\right)\int_{\lambda=0}^{\lambda=1} \frac{\phi^2\psi}{(1+\kappa_{ads}\psi)^2}\,d\lambda$$

$$= \left(\frac{\kappa_{diff}}{\alpha\epsilon}\right)\int_{\lambda=0}^{\lambda=1} \frac{d^2\psi}{d\lambda^2}\,d\lambda$$

$$= \left(\frac{\kappa_{diff}}{\alpha\epsilon}\right)\left[\frac{d\psi}{d\lambda}\right]_{\lambda=1} \quad \text{using boundary condition} \left[\frac{d\psi}{d\lambda}\right]_{\lambda=0} = 0$$